Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Electronic structure, transport properties, and excited states in CoTiSb, CoZrSb, and CoHfSb half-Heusler compounds[1] ANDERSON JANOTTI, ZHIGANG GUI, University of Delaware, Department of Materials Science and Engineering, JASON KAWASAKI, Kavli Institute at Cornell for Nanoscale Science, Cornell University, CHRIS PALMSTROM, Materials Department, University of California, Santa Barbara, BURAK HIMMETOGLU, Center for Scientific Computing, University of California, Santa Barbara — CoTiSb is a member of a large family of half-Heusler compounds with 18 valence electrons. CoTiSb is semiconductor material with a band gap a little over 1 eV, and it has been considered promising for thermoelectric applications. It can be grown on conventional III-V semiconductors, and could potentially be integrated in III-V devices. Here we present results of first-principles calculations of electronic structure, transport properties, and excited states in CoTiSb, as well as CoZrSb and CoHfSb. Electronic structures are studied using density functional theory within the local density approximation, hybrid functional and quasiparticle GW methods. Both room-temperature Seebeck coefficient and carrier mobility are calculated from first-principles. We also determine the band alignments to III-V semiconductors, and all the results are presented and discussed in the light of available experimental data.

[1]This work was supported by the DOE.

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Date submitted: 06 Nov 2015 Electronic form version 1.4